1-methoxypropan-2-yl 2-methylpropanoate 5436-79-3 | DTXSID40281472

3436-79-3	D1721D40201472	

Model Performance

Model	Data

Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 2.31

Global applicability domain: Inside

Local applicability domain index: 5.98e-01

Confidence level: 7.34e-01

Nearest Neighbors from the Training Set

Image not found

2-Isopropyl-6-methyl-4-

pyrimidone

Measured: 1.82 Predicted: 2.23

Image not found

Paraldehyde

Measured: 3.02 Predicted: 2.77

Image not found

4-IsobutyImorpholine

Measured: 1.78 Predicted: 2.69

Image not found

Dimethoate
Measured: 1.58
Predicted: 1.88

Image not found

2,2-Bis(bromomethyl)-1,3-

propanediol Measured: 4.79 Predicted: 3.35